SAMPLE

PROJECT ACCOMPLISHMENTS SUMMARY

CRADA Title:	**Supercomputer Simulation Model for Residual Oil Hydroprocessing Reactors**
CRADA Number:	**LA92C10049**
DOE TTI Number:	**92-MULT-057-B1**
Industrial Partner:	**Amoco Oil Company**

BACKGROUND

In the highly competitive US oil refining industry, engineers are constantly seeking ways to improve the efficiency and reliability of chemical reactors used in various stages of refining. Because of the very large volumes of production involved, small increments in the conversion efficiency, or improvements in reliability (reduced down-time) can frequently add up to large increments in profitability. Hence the stakes are high, and engineers are constantly on the alert for advances in technology that can assist in their efforts to improve existing refining processes.

One such technology is known as Computational Fluid Dynamics (CFD): a field in which scientists and engineers use supercomputers to solve the complex equations of fluid flow in order to help them understand a great many fluid-flow processes that are employed in industry. In oil refining the chemical reactors used often must handle so-called multiphase flows, such as a bed of solid catalyst grains fluidized by the upward flow of a reactive gas or liquid. The resulting motions are called turbulent because of the chaotic appearance to the eye a pot of rapidly boiling water provides a common image of this turbulence.

Hence, the technology of concern here is CFD applied to multiphase turbulent flows. This is of interest to Amoco as a tool for engineering purposes important to its business; the same technology is of interest to DOE because of its use, for example, in improving the quality of plutonium separation processes. The technology is equally useful for addressing a variety of questions in ongoing DOE laboratory experiments and in weapons physics.

In the early 1990s, Amoco Oil Company realized that multiphase CFD was emerging as a potentially valuable analysis tool that could be of considerable benefit to its business goals, if CFD was to be consolidated into a computer code usable by Amoco engineers. Because CFD and multiphase flow theory are two subjects in which LANL has well-established expertise, Amoco approached LANL with a proposal for a cooperative research program aimed at developing a code for multiphase CFD. Since CFD and multiphase flow problems are high on the list of items important to the DOE nuclear weapons mission, the proposal was viewed as quite relevant, and was selected for support under the Technology Transfer Initiative (TTI). Because the LANL expertise is primarily from the theoretical side, and the Amoco expertise primarily from the experimental side, the partnership was expected to yield significant benefits to both partners which could not have been derived by separate research programs.

Summary Note: General purpose code development is a long-term ongoing process, particularly when theoretical model development and model validation work is overlaid with the computer science aspects of modern supercomputing. The work performed during this CRADA project has laid a solid foundation for the extension and continuation of this long-term process. The CRADA work commenced in August 1992 and operated under TTI

funding until September 1994. DOE/Fossil Energy recognized the value of the foundation and elected to fund follow-on work that resulted in an even wider use of CFDLIB in the US oil refining industry. The CRADA continued under DOE/FE sponsorshop with an expanded set of tasks, until completion in October 1996.

DESCRIPTION

The goal of the work was to advance the ability of chemical engineers to analyze complex fluid flows arising in the US oil refining industry. This was to be accomplished by developing a reliable computational tool that utilizes the latest advances in supercomputer architecture for analysis and design of fluidized-bed chemical reactors. The initial Amoco application of the tool was the so-called Residual oil Hydroprocessing Unit (RHU) that converts heavy, high-sulfur residual crude oil into a synthetic crude oil that can be used to produce gasoline and other high-value products. The resulting computer code was expected to have broad applicability to a variety of chemical reactor flows, not only for Amoco purposes, but for applications of other oil refiners as well.

The LANL Computational Fluid Dynamics LIBrary, CFDLIB, was identified as the starting place for creation of the simulation model developed under this CRADA. Generally the work was to enhance this code library by porting to parallel computers, enabling functionality for 3-D simulations, and benchmarking models for the complex physics of turbulent multiphase flows encountered in oil refining processes. The labor was generally divided such that LANL conducted the code development and theory development activities; and Amoco designed and carried out laboratory experiments directed toward producing important data for validation of the LANL theory. Together both Amoco and LANL applied the code to problems such as the RHU as a means of gaining confidence in its use for such applications.

The main results of this work are twofold: first a major leap forward was made in the multiphase CFD analysis capabilities embodied in CFDLIB; and second, the ability for engineers to execute CFDLIB on any modern supercomputer was enabled. The long term implications of these results are important. The first means that a vehicle now exists for examining industrial multiphase flow problems in ways never before possible. Whereas the theory will likely never be complete, good answers to many important questions can be obtained; and the same vehicle can be used to test and develop new and better theories. The second result is that no matter what evolutionary path computer hardware may take in the next decade or so, the same computational vehicle can be used. Care was taken during the project to guarantee portability among computers, rather than designing a code capable of execution on a single type of computer.

The results of the project are expected to have a lasting value; in effect a living vehicle has been created that can be readily updated with current theoretical developments, as well as those that are rapidly occurring in computer science.

ECONOMIC IMPACT

The main economic impact of the work, so far, has been on the Amoco Oil Company. Broader impact could be achieved with additional emphasis on technology transition to other oil refiners and to industries such as chemicals manufacturing, that can make use of modern multiphase CFD simulations. One tangible impact so far for Amoco has been a $5,000,000 capital expenditure savings realized as a result of flow analysis on a liquid-liquid separator unit using CFDLIB. The analysis was performed in June of 1995, by Amoco researchers, with consultation from LANL colleagues.

During the course of the CRADA work, Amoco used the CFDLIB tool for a variety of other refinery-based flow problems. Some of this peripheral work was helpful to Amoco in ways that were not anticipated at the outset. For example, Amoco engineers were able to conceive of improvements to certain gas-liquid separator equipment used in the RHU. These improvements were followed up by Amoco application for US Patents covering the new geometries.

CFDLIB is now being made available to DOE Laboratories, US companies and US universities for a wide variety of engineering and research projects. Among industrial users are Alcoa Aluminum, Boeing Defense and Space Group, Dow Chemical, DuPont, Fluent Inc., Molten Metal Technology, Procter & Gamble, Shell, and Universal Oil Products. Academic users include Colorado State University, Dartmouth College, North Carolina State, University of Utah, UCLA, and Washington University. DOE laboratory users include many groups at LANL, Sandia National Laboratory, Idaho National Engineering Laboratory, and Morgantown Energy Technology Center.

BENEFITS TO DOE

One of the great benefits to DOE resulting from the joint work with Amoco is the experimental data used for model development and validation. This is a direct monetary benefit because DOE can completely avoid the high cost of designing, constructing, and operating laboratory facilities such as those created at Amoco for this project. Clearly this kind of partnering has resulted in important cost-savings for both DOE and for Amoco.

Furthermore, it is now very clear that multiphase CFD represents a true dual-use technology. The industrial and academic uses span applications ranging from molten metal processing to chemicals manufacturing to consumer products process design. Department of Energy applications are similarly broad in nature. Current uses involve simulation of molten salt precipitation processes used for separation of plutonium from handling equipment. Powder casting processes are also being examined with CFDLIB. Also, a large number of ongoing applications related to the engineering of test facilities, such as containment vessels used in laboratory tests, have utilized the new CFDLIB capabilities developed in this project.

The ability to handle these highly beneficial spin-off applications is a natural consequence of our having developed a general-purpose code library rather than a very specialized-purpose code that may address only a single problem. Whereas specialized codes have an important purpose in science and certain engineering applications, our vision was to keep CFDLIB a very general fluid dynamics code collection so that the breadth of usage would be correspondingly wide.

PROJECT STATUS

The CRADA officially closed in October 1996, with all milestones accomplished.

DOE FACILITY POINT OF CONTACT FOR PROJECT INFORMATION

LANL Contact: Bryan A. Kashiwa
Phone: (505) 667-8812
Fax: (505) 665-5926
Address: Group T-3, MS B216
Los Alamos National Laboratory
Los Alamos, New Mexico 87545
E-mail: bak@lanl.gov

COMPANY SIZE AND POINT(S) OF CONTACT FOR PROJECT INFORMATION

Amoco Oil Company is based in Chicago, Illinois.
The company employs approximately 42,000 people.
1996 earnings were posted as $36.1 billion.

Company Contact: Ms. Linda Cadwell
RHU Research Specialist
Phone: (219) 473-3155
Fax: (219) 473-3168
Address: Amoco-Whiting Refinery
2815 Indianapolis Blvd., MC 305
Whiting, IN 46394
E-mail: lacadwell@amoco.com

PROJECT EXAMPLES

One example of how Amoco engineers have used CFDLIB to assist in analysis of oil refining process problems is given in the attached CRADA success story (LALP-94-188, January 1995).

RELEASE OF INFORMATION

Ken Freese, DPPM Program Manager Phone: (505) 665-9090
Fax: (505) 665-0154

Approval for general release:

____

Kenneth Freese Date